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Effect of Dzialoshinski-Moriya interaction on thermal entanglement of a mixed-spin chain

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The effect of Dzialoshinski-Moriya (DM) interaction on thermal entanglement of a mixed-spin chain in an external magnetic field is investigated. It is found that DM interaction may enhance quantum thermal entanglement to a maximal value even though the magnetic field plays a positive role in shrinking thermal entanglement in the mixed-spin chain. Furthermore, the effect of inhomogeneity of the magnetic field on quantum entanglement is analyzed. Our analysis will shed some light on the understanding of the effect of the DM interaction on thermal entanglement of a mixed-spin chain.

thermal entanglement, a mixed-spin chain, DM interaction

As a valuable resource, quantum entanglement plays an important role in quantum information processing and attracts much attention from physicists both in theory and experiment^[1-9]. Recently, the interest in thermal entanglement is growing. Thermal entanglement refers to quantum entanglement of thermal states and it has been investigated extensively by researchers with various quantum spin chain models^[10–19] because the physically realizable quantum mechanisms are not always at zero temperature but often in a thermal equilibrium, e.g. the initial state in nuclear magnetic resonance (NMR) based quantum computing is a thermal state^[20]. The motive to investigate thermal entanglement of spin chains is to find good properties of spin chains for constructing quantum gates, as well as entanglement engineering. One of interesting problems concerning thermal entanglement is to study the effect of magnetic current on ground state entanglement of a 3-qubit XX spin chain in a homogenous field. In ref. [22], the authors analyzed the effect of the inhomogenous field on thermal entanglement of a 3-qubit XX spin chain. Even though the models under study are similar to each other in the respect of the system size under study, yet their motives are different. The former is to study the effect of the homogenous magnetization current on

Sci China Ser G-Phys Mech Astron | Dec. 2008 | vol. 51 | no. 12 | 1897-1904

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the entanglement of ground states, while the latter is to investigate the effect of the inhomogenous magnetic field on thermal entanglement.

Around 50 years ago, Dzisloshinski and Moriya proposed the anisotropic antisymmetric exchange interaction, Dzialoshinski-Moriya (DM) interaction, to explain the weak ferromagnetism of antiferromagnetic crystals (a-Fe2O3, MnCO3) respectively from phenomenological and microscopic points of view^[23-26]. DM interaction arises from the extension of Anderson's theory of superexchange interaction by including the spin-orbit coupling effect. The effect of DM interaction on thermal entanglement of a 2-qubit spin chain has been analyzed by the authors in refs. [11,27,28]. In ref. [11], the authors studied the critical temperature of entanglement for a 2-qubit XX spin chain with DM interaction and found that DM interaction may increase the critical temperature. The authors in ref. [27] investigated thermal entanglement and teleportation of a 2-qubit XXX spin chain in the presence of DM interaction. It was found in ref. [27] that the DM interaction may excite the entanglement and teleportation fidelity. Ref. [28] is an extension of the analysis in ref. [27] from the 2-qubit XXX spin chain to a 2-qubit XYZ spin chain and found that DM interaction may strengthen the thermal entanglement. For an inorganic compound, the quasi-one-dimensional bimetallic chains ACu(pbaOH)(H₂O₃)·2H₂O₃ with each unit cell containing two different spins (S, 1/2), have been synthesized^[29]. The compounds of ACu may be considered as a Heisenberg mixed-spin (S, 1/2) chain with antiferromagnetic interactions. The entanglement witness and characteristic temperature of a mixed-spin chain have been analyzed by authors in ref. [30] where they considered the XXX Heisenberg model. The thermal entanglement of a mixed-spin chain with DM interaction has not been studied yet. What are the roles played by DM interaction and the external magnetic field on the thermal entanglement of a mixed-spin chain? To answer this question, we study the effect of DM interaction on thermal entanglement in the real mixed-spin systems under the external magnetic field.

In this paper, we will investigate the thermal entanglement of a mixed-spin chain with DM interaction by using the entanglement measure of negativity.

1 Our model

Here, we consider the nearest-neighbor mixed-spin chain (S, 1/2) with DM interaction and the Hamiltonian is expressed as

$$H = \sum_{i} J(\mathbf{S}_{i} \cdot \mathbf{s}_{i+1}) + (B+h)S_{i}^{z} + (B-h)S_{i+1}^{z} + \mathbf{D} \cdot (\mathbf{S}_{i} \times \mathbf{s}_{i+1}),$$
(1)

where *J* is exchange coupling constant, *B* and *b* are respectively the strengths of homogenous and inhomogeneous external magnetic field, *S* and *s* respectively denote the spin *S* and the spin 1/2 sites, and the last term represents the DM interaction arising from spin-orbit coupling^[23-26]. The exchange coupling constants of J > 0 and J < 0 denote the antiferromagnetic and ferromagnetic case. In this paper, the antiferromagnetic mixed-spin chain with DM interaction is considered. Choosing the DM interaction of D = Dz, we obtain the Hamiltonian of a qutrit-qubit mixed spin chain (1,1/2) in the following expression:

$$H = J(S_1^x s_2^x + S_1^y s_2^y + S_1^z s_2^z) + (B+h)S_1^z + (B-h)s_2^z + D(S_1^x s_2^y - S_1^y s_2^x),$$
(2)

where S_1^{η} ($\eta = x, y, z$) are spin-1 operators and S_2^{ς} , ($\varsigma = x, y, z$) are familiar Pauli matrices,

$$S_{1}^{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad S_{1}^{y} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad S_{1}^{z} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
(3)

To study the thermal entanglement of the mixed-spin chain in eq. (2), we need to calculate the thermal density matrix ρ which takes the expression of $\rho = (e^{-\beta H})/Z$, where β is the inverse of the multiply of temperature *T* and *k*. *k* is the Boltzman constant, that is $\beta = 1/(kT)$. *Z* is the partition function taking the expression of $Z = \text{tr}(e^{-\beta H})$. Now we diagonalize the Hamiltonian to get the density matrix, and the eigenstates of the above Hamiltonian in eq. (2) read as the following expressions with corresponding eigenvalues respectively according to the formula $H |\psi_j\rangle = \lambda_j |\psi_j\rangle$, $(j = 1, 2, \dots, 6)$:

$$H |\psi_{1}\rangle = (J+2B)|\psi_{1}\rangle, \qquad H |\psi_{6}\rangle = (J-2B)|\psi_{6}\rangle, H |\psi_{2}\rangle = (B+h-J+\Lambda^{+})/2|\psi_{2}\rangle, \qquad H |\psi_{3}\rangle = (B+h-J-\Lambda^{+})/2|\psi_{3}\rangle, H |\psi_{4}\rangle = -(B+h+J-\Lambda^{-})/2|\psi_{4}\rangle, \qquad H |\psi_{5}\rangle = -(B+h+J+\Lambda^{-})/2|\psi_{5}\rangle,$$
(4)

where $|\psi_j\rangle$ $(j = 1, 2, \dots, 6)$ take the following expressions:

$$\begin{split} |\psi_{1}\rangle &= |00\rangle, \qquad |\psi_{6}\rangle = |21\rangle, \\ |\psi_{2}\rangle &= C_{2} \left\{ \frac{J+B-3h+\Lambda^{+}}{-2e} |01\rangle + |10\rangle \right\}, \\ |\psi_{3}\rangle &= C_{3} \left\{ \frac{J+B-3h-\Lambda^{+}}{-2e} |01\rangle + |10\rangle \right\}, \\ |\psi_{4}\rangle &= C_{4} \left\{ \frac{J-B+3h+\Lambda^{-}}{2e} |11\rangle + |20\rangle \right\}, \\ |\psi_{5}\rangle &= C_{5} \left\{ \frac{J-B+3h-\Lambda^{-}}{2e} |11\rangle + |20\rangle \right\}. \end{split}$$

$$(5)$$

In eqs. (4) and (5), Λ^+ , Λ^- take the following expressions:

$$\Lambda^{\pm} = \left\{ \left[J \pm (B - 3h) \right]^2 + 4de \right\}^{\frac{1}{2}},\tag{6}$$

where $d = \sqrt{2}(J + iD)$, $e = \sqrt{2}(J - iD)$, and C_2 , C_3 , C_4 , C_5 are the normalization coefficients for quantum states of $|\psi_2\rangle$, $|\psi_3\rangle$, $|\psi_4\rangle$, $|\psi_5\rangle$, respectively. With the above equations, we get the thermal density matrix in the following form:

$$\rho = e^{-\beta H} / Z = \frac{1}{Z} \begin{pmatrix} M_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & M_{22} & M_{23} & 0 & 0 & 0 \\ 0 & M_{32} & M_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & M_{44} & M_{45} & 0 \\ 0 & 0 & 0 & M_{54} & M_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & M_{66} \end{pmatrix},$$
(7)

MA XiaoSan et al. Sci China Ser G-Phys Mech Astron | Dec. 2008 | vol. 51 | no. 12 | **1897-1904 1899**

where the elements of the density matrix M_{jk} $(j, k = 1, 2, \dots, 6)$ take the expressions of the parameters above and they read

$$\begin{split} M_{11} &= \exp(-\beta\lambda_{1}), \qquad M_{66} = \exp(-\beta\lambda_{6}), \\ M_{22} &= \left|C_{2}\right|^{2} \frac{(1+\sin\theta_{1})^{2}}{\cos^{2}\theta_{1}} \exp(-\beta\lambda_{2}) + \left|C_{3}\right|^{2} \frac{(1-\sin\theta_{1})^{2}}{\cos^{2}\theta_{1}} \exp(-\beta\lambda_{3}), \\ M_{33} &= \left|C_{2}\right|^{2} \exp(-\beta\lambda_{2}) + \left|C_{3}\right|^{2} \exp(-\beta\lambda_{3}), \\ M_{44} &= \left|C_{4}\right|^{2} \frac{(1+\sin\theta_{2})^{2}}{\cos^{2}\theta_{2}} \exp(-\beta\lambda_{4}) + \left|C_{5}\right|^{2} \frac{(1-\sin\theta_{2})^{2}}{\cos^{2}\theta_{2}} \exp(-\beta\lambda_{5}), \\ M_{55} &= \left|C_{4}\right|^{2} \exp(-\beta\lambda_{4}) + \left|C_{5}\right|^{2} \exp(-\beta\lambda_{5}), \\ M_{23} &= M_{32}^{*} = -\left|C_{2}\right|^{2} \frac{1+\sin\theta_{1}}{\cos\theta_{1}} \exp(i\theta - \beta\lambda_{2}) - \left|C_{3}\right|^{2} \frac{\sin\theta_{1}-1}{\cos\theta_{1}} \exp(i\theta - \beta\lambda_{3}), \\ M_{45} &= M_{54}^{*} = \left|C_{4}\right|^{2} \frac{1+\sin\theta_{2}}{\cos\theta_{2}} \exp(i\theta - \beta\lambda_{4}) + \left|C_{5}\right|^{2} \frac{\sin\theta_{2}-1}{\cos\theta_{2}} \exp(i\theta - \beta\lambda_{5}), \end{split}$$
(8)

where θ_1 , θ_2 , θ are defined by the listed equations of $\theta_1 = \arctan\left(\frac{J+B-3h}{\sqrt{8(J^2+D^2)}}\right)$,

$$\theta_2 = \arctan\left(\frac{J-B+3h}{\sqrt{8(J^2+D^2)}}\right)$$
, and $\theta = \arctan\left(\frac{D}{J}\right)$

Let us make some discussion about the entanglement of the ground state of the Hamiltonian in eq. (2). When D takes a value large enough, the ground state is $|\psi_5\rangle$ with an approximate expression of $(-i|11\rangle+|20\rangle)/\sqrt{2}$, the entanglement of which is 0.5 when the negativity is used to measure entanglement. However, the eigenvalue of state $|\psi_3\rangle$ is very close to that of state $|\psi_5\rangle$, and the value of entanglement of state $|\psi_3\rangle$ is 0.5 approximately when the DM interaction is strong enough. Numerical calculation implies that the entanglement of a mixed state consisting of both ensembles of $|\psi_3\rangle$ and $|\psi_5\rangle$ takes a value less than 0.5. When the homogenous or inhomogenous magnetic field is strong enough, the ground state will become a separable state with an approximate expression of $|21\rangle$ or $|20\rangle$. From the heuristic analysis, we find that the DM interaction may enhance thermal entanglement, while the magnetic field, either homogenous or inhomogenous, plays a positive role in shrinking thermal entanglement.

2 Results and discussion

In this paper, we employ negativity as an entanglement measure to analyze our model. As a quantity, negativity was proposed by Zyczkowski and coworkers^[31] with the Peres' criterion for separability^[32], and formulated by Vidal in ref. [33] to measure quantum entanglement of both pure and mixed states. It is known that the Peres' criterion is necessary and sufficient for quantum states of 2×2 and 2×3 systems. In this paper, the density matrix represents the states of a 2×3 system, so negativity may be used to measure the thermal entanglement of the system of concern sufficiently. For a given bipartite density matrix ρ_{AB} , negativity is defined by the following equation:

$$N(\rho_{AB}) = \frac{\|\rho^{T_A}\| - 1}{2},$$
(9)

where $\|\rho^{T_A}\|$ is the sum of the absolute value of the eigenvalues of ρ^{T_A} , and ρ^{T_A} is the partial transpose of the density matrix ρ_{AB} . The partial transpose keeps the trace unchangeable, so negativity is equal to the sum of the absolute value of the negative eigenvalues of ρ^{T_A} and is used to measure the extent to which the partially transposed density matrix fails to be positive. With the above density matrix of concern, the negativity takes the following expression:

$$N(\rho) = \begin{cases} \Omega_{1} + \Omega_{2}, (M_{33} + M_{66} \leq \Delta_{1}, M_{11} + M_{44} \leq \Delta_{2}), \\ \Omega_{1}, (M_{33} + M_{66} \leq \Delta_{1}, M_{11} + M_{44} \geq \Delta_{2}), \\ \Omega_{2}, (M_{33} + M_{66} \geq \Delta_{1}, M_{11} + M_{44} \leq \Delta_{2}), \\ 0, (M_{33} + M_{66} \geq \Delta_{1}, M_{11} + M_{44} \geq \Delta_{2}), \end{cases}$$
(10)

where $\Omega_1, \Omega_2, \Delta_1, \Delta_2$ take the expressions in the following equations:

$$\Omega_{1} = \frac{\Delta_{1} - M_{33} - M_{66}}{2Z}, \qquad \Omega_{2} = \frac{\Delta_{2} - M_{11} - M_{44}}{2Z},$$

$$\Delta_{1} = \sqrt{(M_{33} - M_{66})^{2} - 4|M_{45}|^{2}}, \qquad \Delta_{2} = \sqrt{(M_{11} - M_{44})^{2} - 4|M_{23}|^{2}}.$$
 (11)

From sec. 1, we easily find that the analytical results involve so many parameters and they cannot be expressed as the obvious expression of parameters of *J*, *B*, *h*, *D*, β easily. Fortunately, numerical simulation can demonstrate the results, so in this section, we will analyze the results by using numerical simulation.

In this paper, we concentrate ourselves on the case of antiferromagnetic J = 1. Firstly, we numerically calculate the thermal entanglement of the mixed-spin chain with DM interaction. Let the magnetic field be a constant, that is B = 1, h = 0.1, and we demonstrate the first observation in Figure 1, from which we find that the role played by the DM interaction is to increase quantum



Figure 1 Negativity $N(\rho)$ versus the strength of DM interaction D is plotted under different temperatures, where J = 1, B = 1, h = 0.1.

MA XiaoSan et al. Sci China Ser G-Phys Mech Astron | Dec. 2008 | vol. 51 | no. 12 | 1897-1904 1901

entanglement of the mixed-spin chain. Without DM interaction, that is D = 0, we find that the entanglement of the mixed-spin chain varies with different temperatures. The higher the temperature is, the smaller the amount of the entanglement is. For the cases of low temperatures $\beta = 1, 2, 10$, the thermal entanglement may be enhanced to a stable value when the strength of DM interaction needs only take small values; while for the cases of high temperatures $\beta = 0.2, 0.5$, only the DM interaction takes a large value can the entanglement reach a stable value. The further numerical calculation implies that the stable values of entanglement for the above cases are different from each other. The higher the temperature is, the smaller the stable value of entanglement is. This observation is consistent with our forehead analysis.

To demonstrate the role played by the homogenous magnetic field, we plot Figure 2 to describe the behaviors for quantum entanglement of the mixed-spin chain under different strengths of the homogenous magnetic field. Similarly, we set J = 1, D = 1 and h = 0.1 and plot the cases for entanglement versus the homogenous magnetic field for the mixed-spin chain under different temperatures. From Figure 2, we easily find that the homogenous magnetic field plays a negative role in enhancing quantum entanglement of the mixed-spin chain. The larger the absolute value of the magnetic field is, the smaller the amount of quantum entanglement in the mixed-spin chain is. Even though the quantum entanglement does not decrease monotonically because of some revivals, yet the quantum entanglement will go to zero when the value of the magnetic field is large enough. In the context, we also find a region where the entanglement is enhanced as seen in Figure 2 when the absolute value of |B| ranges from 0 to 1.5 for the cases $\beta = 5$, $\beta = 10$. Specially, the entanglement for the cases with low temperatures $\beta = 5.10$ decreases sharply when the absolute value of the homogenous magnetic field takes a value around 2.5, while for the cases with high temperatures $\beta = 0.5, 0.8, 3$, the entanglement decreases smoothly. We also find this point from the Hamiltonian of the mixed spin chain. When the magnetic field takes large values, the Hamiltonian can be diagonalized approximately with the basis $|\mu\nu\rangle$ ($\mu = 0, 1, 2, \nu = 0, 1$) as eigenvectors, and the density matrix can be approximately considered as a diagonal matrix. It is known that the diagonal density matrix is separable, and the entanglement of a diagonal density



Figure 2 Negativity $N(\rho)$ versus the homogenous magnetic field *B* is plotted under different temperatures, where J = 1, D = 1, h = 0.1.

1902 MA XiaoSan et al. Sci China Ser G-Phys Mech Astron | Dec. 2008 | vol. 51 | no. 12 | 1897-1904

matrix is zero.

Finally, we should consider the effect of the inhomogeneity of the magnetic field on quantum entanglement for the mixed-spin chain. From Figure 3, we find that the entanglement may be enhanced to a maximum with *h* taking a certain finite value and then is decreased to zero with *h* taking a value large enough. The higher the temperature is, the smaller the maximum of the entanglement is. Getting a further insight into Figure 3, we find that the lower the temperature is, the smaller the absolute value of *h* is needed to enhance the entanglement to a maximum. However, when the inhomogenous magnetic field *h* is strong enough, the entanglement will vanish completely. Additionally, we find that the maximum values of entanglement are larger for h > 0 than those for h < 0.



Figure 3 Negativity $N(\rho)$ versus the inhomogenous magnetic field *h* is plotted under different temperatures, where J = 1, B = 1, D = 1.

3 Conclusions

We analyzed the effect of DM interaction on thermal entanglement of a mixed-spin chain under both homogenous and inhomogenous magnetic fields. Our results imply that the entanglement may be enhanced by DM interaction to a stable value which varies with different temperatures. The higher the temperature is, the smaller the stable value is and the larger the value of DM interaction is needed to enhance thermal entanglement of the mixed spin chain to a maximum. Compared to the positive role played by DM interaction in enhancing thermal entanglement, the role played by the magnetic field with large values is negative in enhancing thermal entanglement. For the cases with low temperatures, the entanglement may be enhanced by the homogenous magnetic field taking an absolute value under a certain value. For the cases with high temperatures, the entanglement is decreased with the increasing absolute value of the magnetic field. When the homogenous magnetic field is strong enough, the entanglement completely vanishes for the cases either with high or low temperatures. The inhomogenous magnetic field plays a similar role in enhancing thermal entanglement to the homogenous magnetic field plays a similar role in enhancing thermal entanglement to the homogenous even though their behaviors have some differences. In a word, we think our analysis will shed some light on the effect of DM interaction on thermal entanglement of a mixed-spin chain.

MA XiaoSan et al. Sci China Ser G-Phys Mech Astron | Dec. 2008 | vol. 51 | no. 12 | 1897-1904 1903

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1904 MA XiaoSan et al. Sci China Ser G-Phys Mech Astron | Dec. 2008 | vol. 51 | no. 12 | 1897-1904